6,8-Diazaspiro[3.5]nonane-5,7,9-trione

Other names: cyclobutyl-5-spirobarbituric acid
Inchi: InChI=1S/C7H8N2O3/c10-4-7(2-1-3-7)5(11)9-6(12)8-4/h1-3H2,(H2,8,9,10,11,12)
InchiKey: VQDXQNNYGSEHPU-UHFFFAOYSA-N
Formula: C7H8N2O3
SMILES: O=C1NC(=O)C2(CCC2)C(=O)N1
Mol. weight [g/mol]: 168.15

Physical Properties

Property code	Value	Unit	Source
gf	-96.87	kJ/mol	Joback Method
hf	-362.59	kJ/mol	Joback Method
hfus	14.20	kJ/mol	Joback Method
hvap	56.93	kJ/mol	Joback Method
log10ws	-1.65		Aqueous Solubility Prediction Method
log10ws	-1.66		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-1.66		Estimated Solubility Method
logp	-0.477		Crippen Method
mcvol	112.440	ml/mol	McGowan Method
pc	5721.86	kPa	Joback Method
tb	691.32	K	Joback Method
tc	983.15	K	Joback Method
tf	636.83	K	Joback Method
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.52	J/mol×K	691.32	Joback Method
cpg	333.24	J/mol×K	739.96	Joback Method
cpg	348.19	J/mol×K	788.60	Joback Method
cpg	362.42	J/mol×K	837.23	Joback Method

cpg	376.01	J/mol×K	885.87	Joback Method
cpg	389.03	J/mol×K	934.51	Joback Method
cpg	401.55	J/mol×K	983.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume